3.2 Basic Theory of Carrier Statistics

3.2.1 Fermi-Dirac and Boltzmann Statistics

Electrons in thermal equilibrium at temperature T_L with a semiconductor lattice obey Fermi-Dirac statistics. That is the probability $f(\varepsilon)$ that an available electron state with energy ε is occupied by an electron is:

$$f(\varepsilon) = \frac{1}{1 + \exp\left(\frac{\varepsilon - E_F}{kT_L}\right)} \tag{3-25}$$

where E_F is a spatially independent reference energy known as the Fermi level and k is Boltzmann's constant.

In the limit, $\varepsilon - E_F >> kT_L$, Equation 3-25 can be approximated as:

$$f(\varepsilon) = \exp\left(\frac{E_F - \varepsilon}{kT_L}\right) \tag{3-26}$$

Statistics based on the use of Equation 3-26 are referred to as Boltzmann statistics [321, 127]. The use of Boltzmann statistics instead of Fermi-Dirac statistics makes subsequent calculations much simpler. The use of Boltzmann statistics is normally justified in semiconductor device theory, but Fermi-Dirac statistics are necessary to account for certain properties of very highly doped (degenerate) materials.

The Fermi-Dirac statistics have been implemented in ATLAS in a similar form to Boltzmann statistics.

The remainder of this section outlines derivations and results for the simpler case of Boltzmann statistics which are the default in ATLAS. You can have ATLAS use Fermi-Dirac statistics by specifying the `FERMIDIRAC` parameter in the `MODEL` statement.

3.2.2 Effective Density of States

Integrating the Fermi-Dirac statistics over a parabolic density of states in the conduction and valence bands, whose energy minimum is located at energies E_C and E_V respectively, yields the following expressions for the electron and hole concentrations:

$$n = N_C F_{1/2}\left(\frac{E_F - E_C}{kT_L}\right) \tag{3-27}$$

$$p = N_V F_{1/2}\left(\frac{E_v - E_F}{kT_L}\right) \tag{3-28}$$

where $F_{1/2}(\eta)$ is referred to as the Fermi-Dirac integral of order 1/2. If Equation 3-26 is a good approximation, then Equations 3-27 and 3-28 can be simplified to

$$n = N_C \exp\left(\frac{E_F - E_C}{kT_L}\right) \tag{3-29}$$

$$p = N_V \exp\left(\frac{E_v - E_F}{kT_L}\right) \tag{3-30}$$

which are referred to as the Boltzmann approximation.

N_C and N_V are referred to as the effective density of states for electrons and holes and are given by:

$$N_C(T_L) = 2\left(\frac{2\pi\, m_e^* kT_L}{h^2}\right)^{\frac{3}{2}} M_c = \left(\frac{T_L}{300}\right)^{\mathrm{NC \cdot F}} \mathrm{NC300} \tag{3-31}$$

$$N_V(T_L) = 2\left(\frac{2\pi\, m_h^* kT_L}{h^2}\right)^{\frac{3}{2}} = \left(\frac{T_L}{300}\right)^{\mathrm{NV \cdot F}} \mathrm{NV300} \tag{3-32}$$

where M_c is the number of equivalent conduction band minima. `NC300` and `NV300` are user-definable on the `MATERIAL` statement as shown in Table 3-1.

In some circumstances, the lattice temperature, T_L, is replaced by the electron temperature, T_n, in Equation 3-31 and hole temperature, T_p, in Equation 3-32.

Table 3-1 User-Definable Parameters for the Density of States

Statement	Parameter	Default	Units
MATERIAL	NC300	2.8×10^{19}	cm^{-3}
MATERIAL	NV300	1.04×10^{19}	cm^{-3}
MATERIAL	NC.F	1.5	
MATERIAL	NV.F	1.5	

3.2.3 Intrinsic Carrier Concentration

Multiplying Equations 3-29 and 3-30 yields:

$$np = n_{ie}^2 \tag{3-33}$$

where n_{ie} is the intrinsic carrier concentration and is given for Boltzmann statistics by:

$$n_{ie} = \sqrt{N_C N_V} \exp\left(\frac{-E_g}{2kT_L}\right) \tag{3-34}$$

$E_g = E_C - E_V$ is the band-gap energy.

For intrinsic (undoped) material, $p = n$. By equating Equations 3-29 and 3-30 and solving for E_F yields:

$$E_F = E_i = -q\psi_i = \frac{E_C + E_V}{2} + \left(\frac{kT_L}{2}\right)\ln\left(\frac{N_v}{N_c}\right) \tag{3-35}$$

where E_i is the Fermi level for intrinsic doped silicon, and ψ_i is the intrinsic potential. Equation 3-35 also defines the intrinsic potential under non-equilibrium conditions. As indicated previously, for ATLAS the ψ used in Equation 3-1 is the intrinsic potential.

The electron and hole concentrations can be expressed in terms of the intrinsic carrier concentration as:

$$n = n_{ie}\exp\left[\frac{q(\psi - \phi_n)}{kT_L}\right] \tag{3-36}$$

$$p = n_{ie}\exp\left[\frac{-q(\psi - \phi_p)}{kT_L}\right] \tag{3-37}$$

where ψ is the intrinsic potential and ϕ is the potential corresponding to the Fermi level (i.e., $E_F = q\phi$).

The expression for intrinsic carrier concentration, n_{ie}, can be generalized to Fermi-Dirac statistics using Equations 3-27 and 3-28. Specifying the `NI.FERMI` parameter in the `MODELS` statement will cause ATLAS to calculate n_{ie} using Fermi-Dirac statistics.

3.2.4 Evaluation of Fermi-Dirac Integrals

In addition to the Fermi-Dirac integral of order $\frac{1}{2}$ as used in Equations 3-27 and 3-28, ATLAS also needs to evaluate the Fermi-Dirac integrals of order $\frac{-3}{2}, \frac{-1}{2}, \frac{3}{2}$. There are simple, quickly calculated, but relatively poor approximations available for these integrals. You can also evaluate them to machine precision; however, the amount of computation required makes the evaluations relatively slow. ATLAS uses a Rational Chebyshev approximation scheme, which is efficient in terms of CPU use and also has accuracy close to the machine precision. In the worst case, the approximation differs from the actual values by 1 part in 10^{10} and is typically much better.